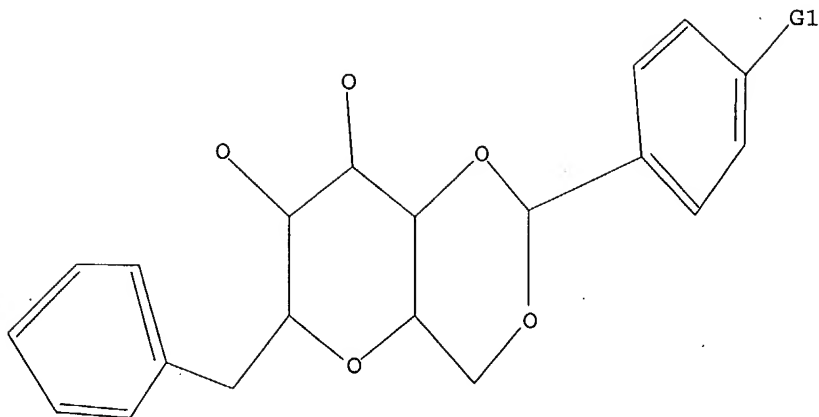


11/01/2004

STR



G1 Cl,Br,F

2 SEA SSS FUL L1

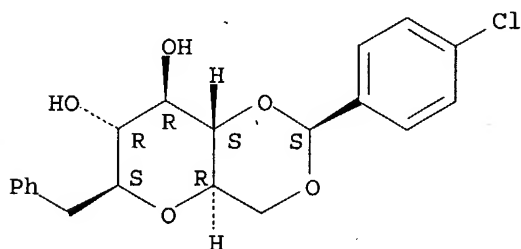
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L2 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 727416-83-3 REGISTRY
 ED Entered STN: 16 Aug 2004
 CN D-glycero-D-gulo-Heptitol, 2,6-anhydro-5,7-O-[(S)-(4-chlorophenyl)methylene]-1-deoxy-1-phenyl- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C20 H21 Cl O5
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
 DT.CA Caplus document type: Patent
 RL.P Roles from patents: PREP (Preparation)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2
C402-C50	OCOC3-OC5	6-6	C7O3	591.449.1	1

Absolute stereochemistry. Rotation (+).



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	973	pH 1	(1) ACD
Bioconc. Factor (BCF)	973	pH 4	(1) ACD
Bioconc. Factor (BCF)	973	pH 7	(1) ACD
Bioconc. Factor (BCF)	973	pH 8	(1) ACD
Bioconc. Factor (BCF)	972	pH 10	(1) ACD
Boiling Point (BP)	565.4+/-50.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (HVP)	89.34+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	295.7+/-54.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	5		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	2		(1) ACD
Koc (KOC)	4789	pH 1	(1) ACD
Koc (KOC)	4789	pH 4	(1) ACD
Koc (KOC)	4789	pH 7	(1) ACD
Koc (KOC)	4789	pH 8	(1) ACD
Koc (KOC)	4784	pH 10	(1) ACD
logD (LOGD)	4.23	pH 1	(1) ACD
logD (LOGD)	4.23	pH 4	(1) ACD
logD (LOGD)	4.23	pH 7	(1) ACD
logD (LOGD)	4.23	pH 8	(1) ACD
logD (LOGD)	4.23	pH 10	(1) ACD
logP (LOGP)	4.235+/-0.521		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	376.83		(1) ACD
pKa (PKA)	12.98+/-0.20	Most Acidic	(1) ACD
Vapor Pressure (VP)	1.28E-13 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

ACCESSION NUMBER: 141:134051 CA
TITLE: Bicyclic carbohydrates as antiprotozoal bioactive for
the treatment of infections caused by parasites
INVENTOR(S): Sas, Benedikt; Van Hemel, Johan; Vandenkerckhove, Jan;
Van Hemel, Johan; Peys, Eric; Van Der Eycken, Johan;
Ruttens, Bart; Van Hoof, Steven
PATENT ASSIGNEE(S): Kemin Pharma Europe B.V.B.A., USA
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
INT. PATENT CLASSIF.:
MAIN: A61K
CLASSIFICATION: 1-5 (Pharmacology)
Section cross-reference(s): 33
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004062590 A2 20040729 WO 2004-US311 20040107

W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AU, AZ, AZ, BA, BB,
BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR,
CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG,
ES, ES, FI, FI, GB, GD, GE, GE, GH, GH, GH, GM, HR, HR, HU, HU,
ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ,
KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN,
MW, MX, MX, MZ

US 2004180838 A1 20040916 US 2004-752792 20040107

PRIORITY APPLN. INFO.: US 2003-438474P 20030107

ABSTRACT:

The use of bicyclic carbohydrates for the treatment of parasite infections is described. Different bicyclic carbohydrates have been tested in vitro against a number of protozoa. These compds. also have been screened against viruses, tumors, bacteria and fungi. Compound A1, a thiophenyl-containing bicyclic carbohydrate possessed significant activity against *Trypanosoma brucei rhodesiense*, a parasite that causes the lethal sleeping sickness. Compound A2 and Compound A3, bicyclic carbohydrates with halogen containing aryl groups, possessed significant activity against *Leishmania donovani*, a parasite that causes leishmaniasis. Bicyclic carbohydrates in general, and Compound A1, Compound A2 and Compound A3 more specifically, could be possible treatments for the sleeping sickness and leishmaniasis in the future.

SUPPL. TERM: bicyclic carbohydrate antiprotozoal parasite infection;
 Trypanosoma brucei rhodesiense inhibition bicyclic
 carbohydrate; *Leishmania donovani* inhibition bicyclic
 carbohydrate

INDEX TERM: Human
 Leishmania
 Leishmania donovani
 Mammalia
 Parasite
 Protozoa
 Protozoacides
 Trypanosoma
 Trypanosoma rhodesiense
 Trypanosomicides

(bicyclic carbohydrates as antiprotozoal agent for
treatment of parasite infections)

INDEX TERM: Carbohydrates, biological studies

ROLE: BSU (Biological study, unclassified); PAC
(Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(bicyclic; bicyclic carbohydrates as antiprotozoal agent
for treatment of parasite infections)

INDEX TERM: Leishmania
 (leishmaniasis from; bicyclic carbohydrates as
 antiprotozoal agent for treatment of parasite infections)

INDEX TERM: Protozoacides
 (leishmanicides; bicyclic carbohydrates as antiprotozoal
 agent for treatment of parasite infections)

INDEX TERM: Drug resistance
 (protozoal, treatment of; bicyclic carbohydrates as
 antiprotozoal agent for treatment of parasite infections)

INDEX TERM: Infection
 (protozoal; bicyclic carbohydrates as antiprotozoal agent
 for treatment of parasite infections)

INDEX TERM: Infection
 (trypanosomiasis; bicyclic carbohydrates as antiprotozoal
 agent for treatment of parasite infections)

INDEX TERM: 87508-17-6P 727416-80-0P 727416-82-2P

ROLE: BSU (Biological study, unclassified); PAC
(Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP

(Preparation); USES (Uses)

(bicyclic carbohydrates as antiprotozoal agent for treatment of parasite infections)

INDEX TERM: 727416-83-3P

ROLE: BYP (Byproduct); PREP (Preparation)

(bicyclic carbohydrates as antiprotozoal agent for treatment of parasite infections)

INDEX TERM: 100-58-3, Phenyl magnesium bromide 104-88-1,
p-Chlorobenzaldehyde, reactions 108-98-5, Thiophenol,
reactions 455-19-6 604-69-3, β -D-Glucose
pentaacetate 1125-88-8, Benzaldehyde dimethyl acetal
6921-34-2, Benzylmagnesium chloride 38768-81-9,
2,3,4,6-Tetra-O-benzyl-D-glucose

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(bicyclic carbohydrates as antiprotozoal agent for treatment of parasite infections)

INDEX TERM: 572-09-8P 2936-70-1P 4196-35-4P 13231-13-5P
20181-49-1P 23661-28-1P 136034-23-6P 155590-31-1P
727416-79-7P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(bicyclic carbohydrates as antiprotozoal agent for treatment of parasite infections)

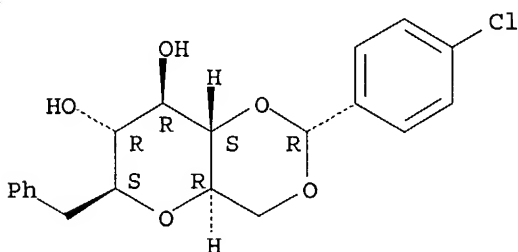
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RN 727416-82-2 REGISTRY
 ED Entered STN: 16 Aug 2004
 CN D-glycero-D-gulo-Heptitol, 2,6-anhydro-5,7-O-[(R)-(4-chlorophenyl)methylene]-1-deoxy-1-phenyl- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C20 H21 Cl O5
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
 DT.CA Caplus document type: Patent
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Absolute stereochemistry. Rotation (-).



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
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Bioconc. Factor (BCF)	973	pH 4	(1) ACD
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 PATENT ASSIGNEE(S): Kemin Pharma Europe B.V.B.A., USA
 SOURCE: PCT Int. Appl., 26 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 INT. PATENT CLASSIF.:
 MAIN: A61K
 CLASSIFICATION: 1-5 (Pharmacology)
 Section cross-reference(s): 33
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004062590	A2	20040729	WO 2004-US311	20040107
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KR, KR, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ				
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PRIORITY APPLN. INFO.:			US 2003-438474P	20030107

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Leishmania donovani
Mammalia
Parasite
Protozoa
Protozoacides
Trypanosoma
Trypanosoma rhodesiense
Trypanosomicides
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(trypanosomiasis; bicyclic carbohydrates as antiprotozoal
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p-Chlorobenzaldehyde, reactions 108-98-5, Thiophenol,
reactions 455-19-6 604-69-3, β -D-Glucose
pentaacetate 1125-88-8, Benzaldehyde dimethyl acetal
6921-34-2, Benzylmagnesium chloride 38768-81-9,
2,3,4,6-Tetra-O-benzyl-D-glucose
ROLE: RCT (Reactant); RACT (Reactant or reagent)
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INDEX TERM: 572-09-8P 2936-70-1P 4196-35-4P 13231-13-5P
20181-49-1P 23661-28-1P 136034-23-6P 155590-31-1P
727416-79-7P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(bicyclic carbohydrates as antiprotozoal agent for
treatment of parasite infections)

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